National Defence / Défense nationale

DEVELOPMENT OF A SINGLE-ZONE DIRECT INJECTION DIESEL ENGINE MODEL

by

W.S. Neill and G.D. Webster
Energy Systems Section
Energy Conversion Division

DEFENCE RESEARCH ESTABLISHMENT OTTAWA
TECHNICAL NOTE 84-12

PCN
25B10

August 1984
Ottawa

ABSTRACT

A computer model is being developed at DREO to simulate the combustion process in diesel engines, and in particular to acquire the ability to predict the effects of future lower grade fuels on diesel engine performance. A baseline thermodynamic model has been completed. Two rate equations developed by Whitehouse and Way, describe the transient fuel/air mixing and reaction kinetic processes. A parametric study was initiated to obtain a better understanding of the sensitivity of fuel parameters and modelling constants on the model's output. It was found that the model produces pressure and heat release diagrams with the correct shape and magnitude. The model predicted the correct trending in all cases studied. In order to use the model as a predictive tool, the effect of engine and fuel variables on the modelling constants will have to be determined.

RÉSUMÉ

On met au point au CRDO un modèle informatisé pour simuler le processus de combustion dans les moteurs diesel et, en particulier, pour pouvoir prévoir les effets des futurs combustibles de basse qualité sur la performance des moteurs diesel. On a terminé un modèle thermodynamique fondamental. Whitehouse et Way ont établi deux équations de débit décrivant le mélange transitoire combustible/air et la cinétique de la réaction. On a entrepris une étude paramétrique dans le but de mieux comprendre comment les paramètres du combustible et les constantes de modélisation influent sur les résultats de modèle. On a observé que le modèle fournissait des diagrammes de pression et de dégagement de chaleur qualitativement et quantitativement corrects. Le modèle prévoit les tendances correctes dans tous les cas étudiés. Afin de pouvoir utiliser le modèle comme outil de prévision, il faudra déterminer les effets des variables du moteur et du combustible sur les constantes de modélisation.

TABLE OF CONTENTS

		PAGE
	ABSTRACT	iii
	RESUME	ii
1.0.0	INTRODUCTION TO DIESEL ENGINE COMBUSTION MODELLING	1
2.0.0	DEVELOPMENT OF A SINGLE-ZONE COMBUSTION MODEL	3
2.1.0	Introduction	3
2.2.0	Thermodynamic Calculations	3
	2.2.1 Polytropic Compression	3
	2.2.2 Energy Equation	4
	2.2.3 Chemical Reaction of a Hydrocarbon Fuel	4
	2.2.4 Internal Energy of the Gases	4
	2.2.5 Work Done by the Gases	5
	2.2.6 Heat Transfer to the Cylinder Walls	5
2.3.0	Combustion Calculations	6
	2.3.1 Introduction	6
	2.3.2 Fuel Preparation Rate Equation	6
	2.3.3 Fuel Reaction Rate Equation	7
2.4.0	Summary of the Single-Zone Combustion Model	8
3.0.0	PARAMETRIC STUDY ON THE SINGLE-ZONE COMBUSTION MODEL	11
3.1.0	Introduction	11
3.2.0	Baseline Data	11
3.3.0	Parameter Variations	12
	3.3.1 Polytropic Compression Index	12
	3.3.2 Injection Timing	12
	3.3.3 Lower Heating Value of the Fuel	12
	3.3.4 Preparation Rate Equation Constant	12
	3.3.5 Apparent Activation Energy of the Fuel	23
4.0.0	FUTURE WORK ON COMBUSTION MODELLING	27
4.1.0	Model Performance Evaluation	27
	CONCLUSIONS	29
	RECOMMENDATIONS	31
	NOMENCLATURE	33
	REFERENCES	35
	APPENDIX A - Calculation of Cylinder Volume	37
	APPENDIX B - Program Listing	39
	APPENDIX C - Input File Required to Run Program	53

1.0.0 INTRODUCTION TO DIESEL ENGINE COMBUSTION MODELLING

Diesel engine combustion models attempt to simulate, to varying degrees, the processes that occur inside the combustion chamber of a diesel engine. These modelling activities contribute towards an increased understanding of the physical processes, determine key controlling variables, and enable one to predict engine behaviour to some extent. Combustion models can be classified into three categories (1):

i) zero-dimensional (single-zone) models,

ii) quasi-dimensional (multi-zone) models, and

iii) multi-dimensional models.

Zero-dimensional combustion models treat the combustion chamber as a single region containing a mixture of gases with one set of bulk properties at any particular time. An energy balance is successively applied to the trapped volume of gases from intake valve closure to exhaust valve opening. The internal energies of the individual component gases are calculated using polynomial functions of temperature. Heat transfer to the cylinder walls can be estimated by experimental measurements, or a correlation developed by Annand (2) or Woschni (3) may be applied. Single-zone models are generally used for one of two purposes:

i) if experimental cylinder pressure as a function of crank angle is input, the model serves to interpret experimental data (eg., calculate apparent heat release), or

ii) if rate equations describing the burning process are input, the model will predict gross engine performance parameters.

Quasi-dimensional diesel engine models predict the rate of burning inside the combustion chamber using more physical quantities than in a zero-dimensional model. However, spatial distribution is not introduced as an independent variable. The cylinder contents are usually divided into a number of compositionally distinct zones. For example, a four zone model (4) might include:

i) a fuel zone,

ii) a stoichiometric fuel-air burning zone,

iii) a product of combustion and hot air zone, and

iv) a cool air zone.

The quasi-dimensional model calculates the movement with time of the various species from one zone to another using physical sub-models for the turbulent combustion process.

Quasi-dimensional models have two major advantages over zero-dimensional models. Firstly, quasi-dimensional models contain a more detailed simulation of the fuel-air mixing process, and are thus able to account for regions of oxygen deficiency. Secondly, the burning zone temperature obtained using a quasi-dimensional model is a realistic temperature from which to estimate pollutant formation.

Multi-dimensional models have both space and time as independent variables. The actual fluid flow in the combustion chamber is simulated using the equations of conservation of mass, momentum, energy and individual species. Because of the complexity of the turbulence, chemical, and boundary-layer processes, certain simplifying assumptions are required to make the problem tractable. The assumptions can be categorized (5) as:

i) dimensional approximations (symmetry, geometrical),

ii) coordinate approximations (Eulerian, Lagrangian),

iii) numerical algorithms/schemes (implicit, explicit), and

iv) theoretical approximations (modelling the processes).

Two general comments can be made about multi-dimensional modelling endeavours. Firstly, extensive experimental measurements of fluid flow must be performed in conjuction with the modelling if meaningful results are to be obtained. Secondly, a simplified approach to reaction kinetics must accompany the more accurate fluid dynamics because of computer limitations.

2.0.0 DEVELOPMENT OF A SINGLE-ZONE COMBUSTION MODEL

2.1.0 INTRODUCTION

A modelling program was undertaken at DREO to:

i) attain a better understanding of combustion in internal combustion engines, and

ii) acquire some predictive capability with regard to fuel effects on diesel engine performance.

Initial efforts were directed towards developing an adaptable baseline thermodynamic model. A single-zone model was selected because of its relative simplicity.

This report summarizes work completed to date on single-zone modelling. In this section, the basic thermodynamic equations used in the model are developed, the two rate equations simulating the combustion process are discussed, and a flowchart of the computer program is presented.

2.2.0 THERMODYNAMIC CALCULATIONS

2.2.1 Polytropic Compression

During the period from intake closure until the start of fuel injection, the gas composition in the combustion chamber is fixed. An energy balance applied to the trapped volume of gases yields:

$$dU = -dW - dQ$$

As an iterative numerical technique is required to solve the above equation, and its solution yields no information about fuel combustion, the process is often approximated to a reversible law of the form PV^n = constant. Using the polytropic compression approximation, and assuming the gaseous mixture to react as a perfect gas, the resulting equations are:

$$P_\theta = P_{ivc} \left(\frac{V_{ivc}}{V_\theta}\right)^n \quad \text{and} \qquad [1a]$$

$$T_\theta = T_{ivc} \left(\frac{V_{ivc}}{V_\theta}\right)^{n-1} \quad \text{for} \quad ivc < \theta \leq inj \qquad [1b]$$

where θ = crank angle (deg)

ivc = intake valve closure (deg)

inj = start of injection (deg)

The calculation of combustion chamber volume as a function of crank angle is presented in Appendix A.

The polytropic index of compression (n) is determined experimentally by measuring the slope of the pressure versus volume plot on the logarithmic scale.

2.2.2 Energy Equation

During the combustion portion of the diesel engine cycle, an energy balance on the trapped gaseous mixture takes the form:

$$dU = \dot{R} d\theta - dQ - dW \qquad [2]$$

where $\dot{R}$ = fuel reaction rate ($\frac{J}{g}$/deg crank angle)

θ = crank angle (deg)

The terms in the energy equation are a function of both temperature and pressure. If the cylinder contents are assumed to behave as a perfect gas mixture, then PV = nRT, and an iterative technique can be used to solve the two equations simultaneously.

2.2.3 Chemical Reaction of a Hydrocarbon Fuel

The complete combustion of a hydrocarbon fuel (C_aH_b) in oxygen (O_2) produces carbon dioxide (CO_2) and water vapour (H_2O) according to the following reaction:

$$C_aH_b + (a + \frac{b}{4})\ O_2 \rightarrow (a)CO_2 + (\frac{b}{2})\ H_2O \qquad [3]$$

If ΔM_f grams of liquid fuel burn completely during a crank angle increment, the decrease in moles of fuel and oxygen are $(\frac{\Delta M_f}{12a+b})$ and $(a + \frac{b}{4})$ $(\frac{\Delta M_f}{12a+b})$ while the increase in moles of carbon dioxide and water vapour are (a) $(\frac{\Delta M_f}{12a+b})$ and $(\frac{b}{2})$ $(\frac{\Delta M_f}{12a+b})$ respectively. Note that the total number of moles of gases in the cylinder increases by $(\frac{b}{4})$ $(\frac{\Delta M_f}{12a+b})$ due to the combustion of the fuel.

2.2.4 Internal Energy of the Gases

The total internal energy of the gases in the control volume is calculated by assuming that the cylinder contents are a mixture of ideal gases. This implies that the total internal energy of the gases is equal to the summation of the individual component internal energies; and that these are only a function of temperature. Benson (6) has tabulated specific internal energies of a number of gases from 0 to 6000 K, and also presents polynomial equations that have been fitted to the data.

Elements are given a reference enthalpy of zero at 0 K. As the lower heating value of fuels are referenced to 298 K, the internal energy of each gas must be referenced to 298 K as follows:

$$U_{298}(T) = U_o(T) - U_o(298) \qquad [4]$$

where the subscript refers to the reference temperature of the internal energy.

2.2.5 Work Done by the Gases

The differential work done by the gases in the combustion chamber on a piston over a differential volume is given by:

$$dW = PdV \qquad [5]$$

where P is the average cylinder pressure over dV. If the volume change is small in going from state 1 to state 2, the previous expression may be linearly approximated by:

$$W_{12} = \left(\frac{P_1 + P_2}{2}\right)(V_2 - V_1) \qquad [6]$$

2.2.6 Heat Transfer to the Cylinder Walls

Many investigators have proposed equations to calculate the instantaneous heat transfer rate to the cylinder walls of reciprocating internal combustion engines. Annand (2) presents a review of several of the existing formulae and suggests that none of them are acceptable. His method, which is used at DREO presently, is to divide the heat transfer up into a convective and a radiative component. Thus:

$$q_{tot} = q_{conv} + q_{rad}$$
$$= h(T - T_w) + c\,(T^4 - T_w^4) \qquad [7]$$

where h and c are the convective and radiative heat transfer coefficients respectively.

The three dimensionless parameters for correlating forced convection heat transfer data are the Nusselt, Reynolds, and Prandtl numbers. Empirical relations usually take the functional form

$$Nu = X\,Re^Y\,Pr^Z \qquad [8]$$

where X, Y and Z are dimensionless constants to be determined experimentally (7). Annand (2) assumes that forced convective heat transfer depends only on the amount of turbulence in the combustion chamber (Z = 0.0). Substituting,

$$h = \frac{k}{D}(Nu) = \frac{k}{D}(X\,Re^Y) \qquad [9]$$

The Reynolds number is based on the mean piston velocity as this provides some indication of the turbulence level in the combustion chamber.

The empirical constants X,Y and c from equations 7 and 8 must be set for combustion modelling applications. Annand (2) determined that the exponent (Y) was approximately 0.70 for a number of diesel engines. The other two constants, X and c, are prescribed such that the total heat transfer amounts to twenty-eight percent (8) of the total fuel energy input and radiation heat transfer accounts for twenty percent of the total heat transfer (3).

A more detailed heat transfer expression has been developed by Woschni (3). His work considers gas motion effected by combustion in addition to general turbulence in the combustion chamber.

2.3.0 COMBUSTION CALCULATIONS

2.3.1 Introduction

Diesel engines are generally designed in such a manner that the initial fuel injected into the combustion chamber does not burn immediately. A sustained chemical reaction will only occur after the cylinder contents have been compressed sufficiently to provide heat for pre-ignition reactions to initiate. Ignition, defined here as the start of rapid pressure rise, usually occurs just a few degrees before top dead centre. Consequently, time is available for fuel to vapourize and a combustible change accumulates. The amount of fuel premixed during the ignition delay period is a function of the fuel injection characteristics, the engine design and the fuel itself. A rapid combustion reaction occurs at ignition, generally burning all of the premixed fuel/air. After the rapid chemical reaction phase, the fuel/air mixing rate controls the reaction rate.

Two rate equations, proposed by Whitehouse and Way (9), describe the combustion process in the single-zone model. The fuel preparation rate equation quantifies the mass of fuel/air mixture that is physically ready for combustion each crank angle degree. The fuel reaction rate equation calculates the mass of prepared fuel that burns with oxygen per crank angle degree. The following sections will discuss the two rate equations in more detail.

2.3.2 Fuel Preparation Rate Equation

The fuel preparation rate equation was developed from the hypothesis that the rate of fuel/air mixing is dependent on the total surface area of the droplets forming the fuel spray. Secondly, oxygen is assumed to surround each droplet. Thirdly, the droplets are assumed to all form into spheres of equal diameter at injection. Finally, fuel/air mixing is also proportional to the amount of oxygen in the combustion chamber. The fuel preparation rate equation proposed by Whitehouse and Way (9) is:

$$\frac{dm_p}{d\theta} = K_p m_i^{1/3} m_u^{2/3} P_{O_2}^{0.4} \qquad [10]$$

where m_p = mass of prepared (mixed) fuel (g)

m_i = mass of injected fuel (g)

m_u = mass of unprepared (unmixed) fuel (g)

P_{O_2} = partial pressure of oxygen (Pa)

K_p = empirical constant

2.3.3 Fuel Reaction Rate Equation

A global reaction rate equation, based on the kinetic theory of gases, is used presently in the single-zone model. The reaction rate equation takes the form:

$$\frac{dm_r}{d\theta} = \text{constant x velocity of gas molecules} \quad \text{x oxygen density x prepared fuel density} \quad \text{x exp (-act/T)} \qquad [11a]$$

where exp(-act/T) represents the fraction of fuel molecules at temperature T which have an energy level greater than the activation energy of the fuel. Two approximations are made to obtain the final form of the equation:

1. The average velocity of the gas molecules is assumed to be proportional to the square root of the average cylinder temperature.

2. Oxygen density is assumed to be proportional to the partial pressure of oxygen divided by the average combustion chamber temperature.

The final form of the fuel reaction rate equation is:

$$\frac{dm_r}{d\theta} = \frac{K_r P_{O_2} m_p}{N T^{\frac{1}{2}}} \exp(-act/T) \qquad [11b]$$

where m_r = mass of fuel burned (g)

m_p = mass of fuel prepared (g)

N = engine speed (rpm)

T = average cylinder temperature (K)

P_{O_2} = partial pressure of oxygen (Pa)

act = activation energy of fuel (K)

K_r = empirical constant

2.4.0 SUMMARY OF THE SINGLE-ZONE COMBUSTION MODEL

A computer program has been written, using Fortran IV, to calculate cylinder pressure, temperature, work done on the piston and apparent heat release as a function of crank angle (see Appendix B). Inputs required to run program include engine dimensions, fuel parameters, a fuel injection schedule, trapped (initial) cylinder conditions and empirical modelling constants (see Appendix C). A flowchart of the model is presented in Figure 1.

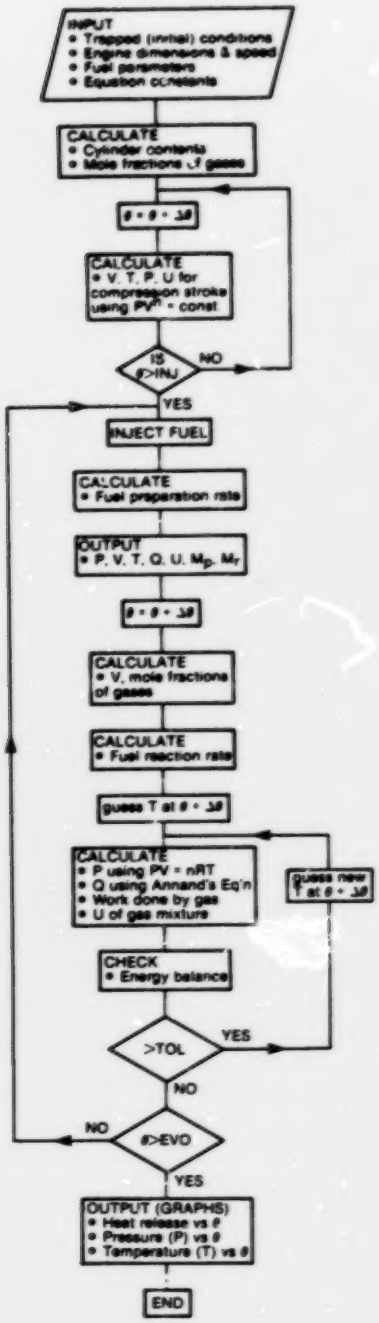


Figure 1. FLOWCHART OF SINGLE-ZONE COMBUSTION MODEL.

3.0.0 PARAMETRIC STUDY ON THE SINGLE-ZONE COMBUSTION MODEL

3.1.0 INTRODUCTION

A parametric study was performed on the single-zone combustion model. The objective was to obtain a better understanding of the sensitivity of both fuel parameters and modelling constants on the predicted performance of a Deutz FIL511D single cylinder diesel engine. Two of the rate equation constants (K_p and act) in the single-zone model were first selected to match the modelled curve to an experimental trace. Then, the fuel and modelling parameters were varied about their baseline values. Note that since K_r and act occur in the same equation, only act was varied.

3.2.0 BASELINE DATA

In order to perform the parametric study, baseline values of the modelling constants had to be established. An experimental test run performed on the Deutz FIL511D single cylinder diesel engine at 1350 rpm, using a 3-GP-30M high stability diesel fuel, was chosen. The following procedure was used to set the preparation rate equation (K_p) and the activation energy (act):

1) The activation energy was varied until the start of rapid pressure rise of the modelled cylinder pressure curve coincided with that of the experimental trace.

2) The preparation rate equation constant was then adjusted until the slope and magnitude of the rapid pressure rise region of the modelled pressure curve was similar to that of the experimental trace.

Baseline values of the modelling parameters that were varied are summarized in Table 1.

PARAMETER		BASELINE VALUE
polytropic compression index	n	1.30
start of injection	inj	-22 °BTDC
lower heating value	LHV	41.0 kJ/g
mixing rate equation constant	K_p	210×10^{-6} -
activation energy	act	14500 K

TABLE 1. Baseline Modelling Parameters

The baseline pressure - crank angle curve is presented in Figure 2a. The maximum cylinder pressure is 8.66 MPa and occurs at 4°ATDC. The maximum rate of pressure rise is 0.95 MPa/degree crank angle and occurs at 6°BTDC. The heat release rate at this position is 150.6 J/degree (Figure 2b).

3.3.0 PARAMETER VARIATIONS

3.3.1 Polytropic Compression Index

The polytropic compression index is used in the single-zone model to simulate the pressure-volume relationship in the combustion chamber during the compression stroke until the start of fuel injection. Increasing the index, while holding all other variables in the model constant, raises the energy level in the combustion chamber during the compression stroke. This tends to reduce the ignition delay because the cylinder contents are able to spontaneously ignite earlier in the cycle. In addition, the maximum rate of heat release is reduced because less fuel mixes during the shorter ignition delay period. The pressure and heat release diagrams are presented in Figure 3.

3.3.2 Injection Timing

The start of fuel injection timing was both advanced and retarded 2° to determine the predicted effect of varying injection timing on the performance of the research engine. Normally, one expects that retarding the fuel injection timing will decrease the time for fuel/air mixing. The rapid combustion reaction will thus be moderated. Figure 4 shows that the maximum rate of heat release is reduced form 185.7 J/crank angle degree to 125.5 J/degree by retarding the timing from 24° to 20° BTDC.

3.3.3 Lower Heating Value of the Fuel

The lower heating value of the diesel fuel was varied ±3 percent of the baseline value of 41.0 kJ/g. This range of heating values was deemed to be typical of those expected from future Canadian Tar Sands derived fuels. The graphs of pressure and heat release versus crank angle in Figure 5 indicate that the variations in heating values of future diesel fuels (not including alternative fuels) will not have a large effect on diesel engine performance.

3.3.4 Preparation Rate Equation Constant (K_p)

The preparation rate equation quantifies the amount of fuel that mixes with air in a stoichiometric rate at each crank angle interval. The physical significance of increasing the preparation rate equation constant is that fuel/air mixing is assumed to occur at a higher rate early in the power stroke. Hence, more fuel accumulates during the ignition delay period. This results in a higher maximum rate of heat release and a higher maximum cylinder pressure (Figure 6).

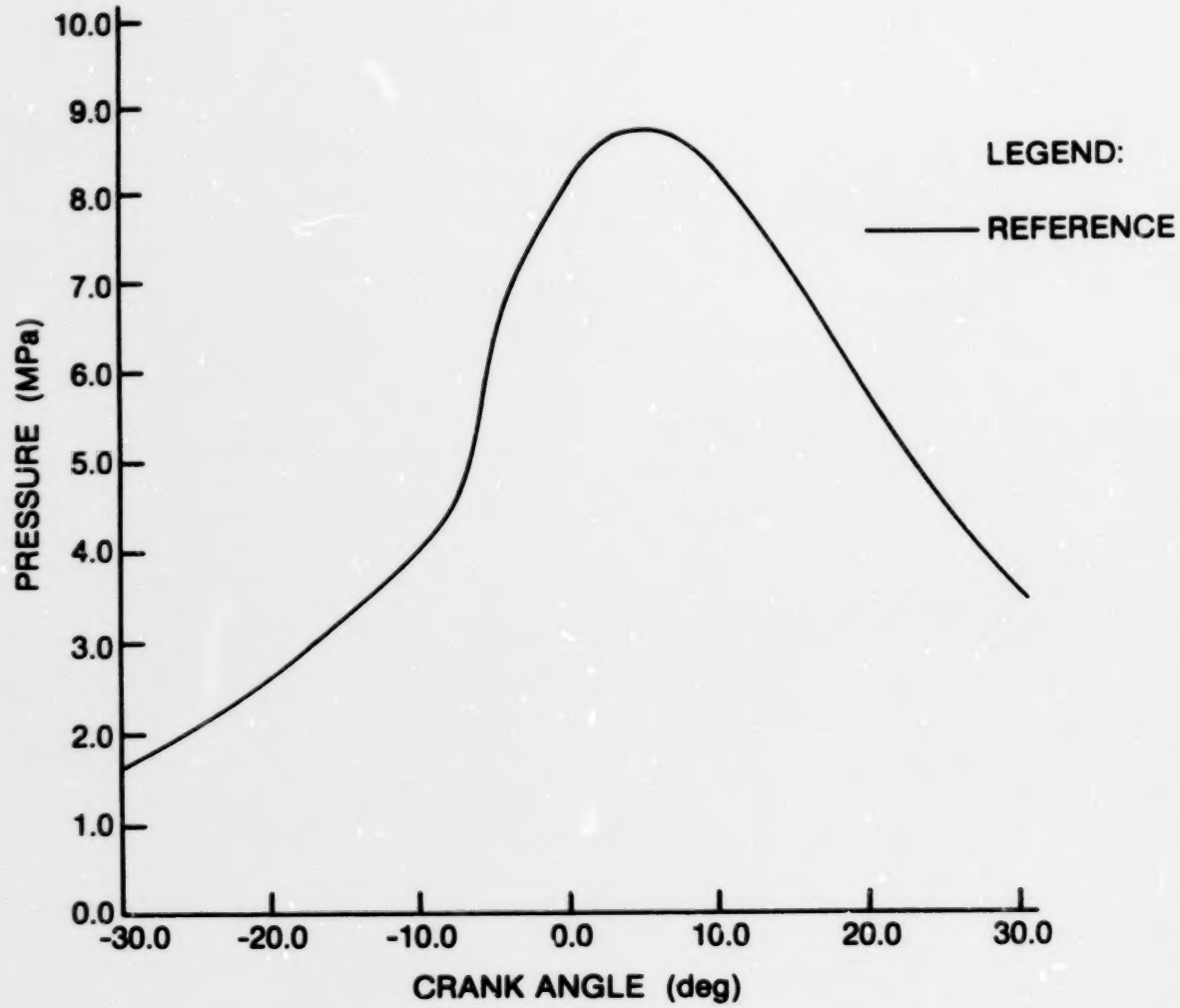


Figure 2(a). BASELINE GRAPH:
CYLINDER PRESSURE VS CRANK ANGLE

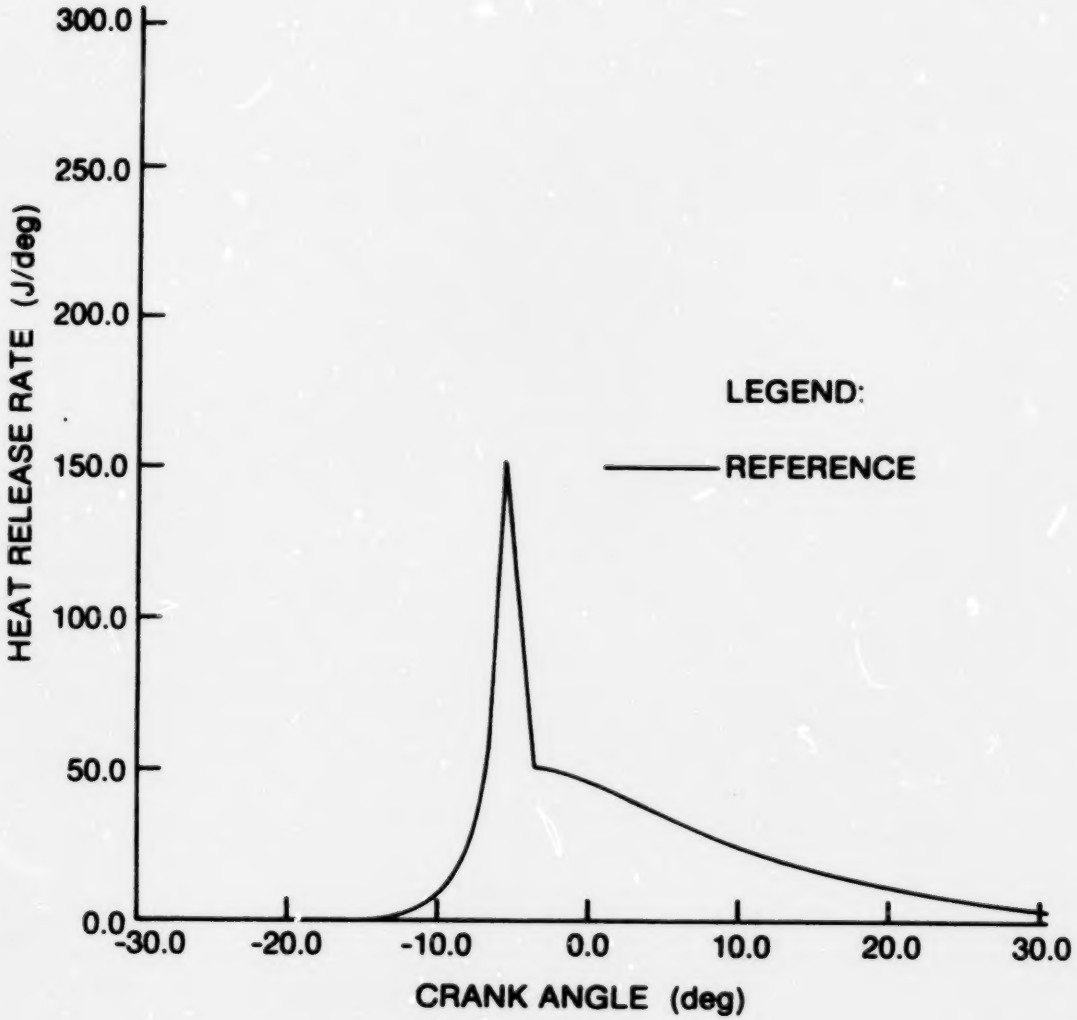


Figure 2(b). BASELINE GRAPH:
HEAT RELEASE RATE VS CRANK ANGLE

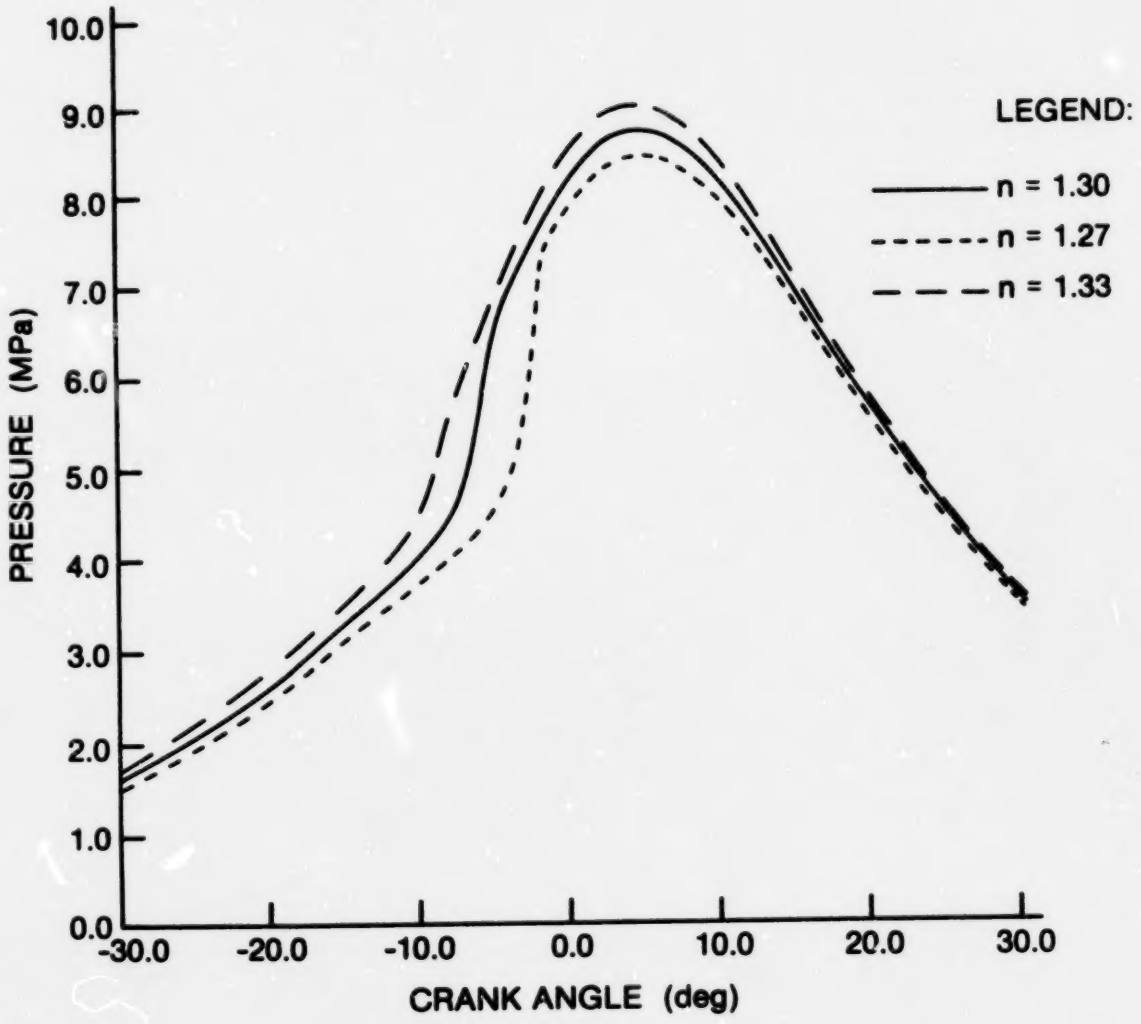


Figure 3 (a). EFFECT OF VARYING THE POLYTROPIC COMPRESSION INDEX: CYLINDER PRESSURE VERSUS CRANK ANGLE.

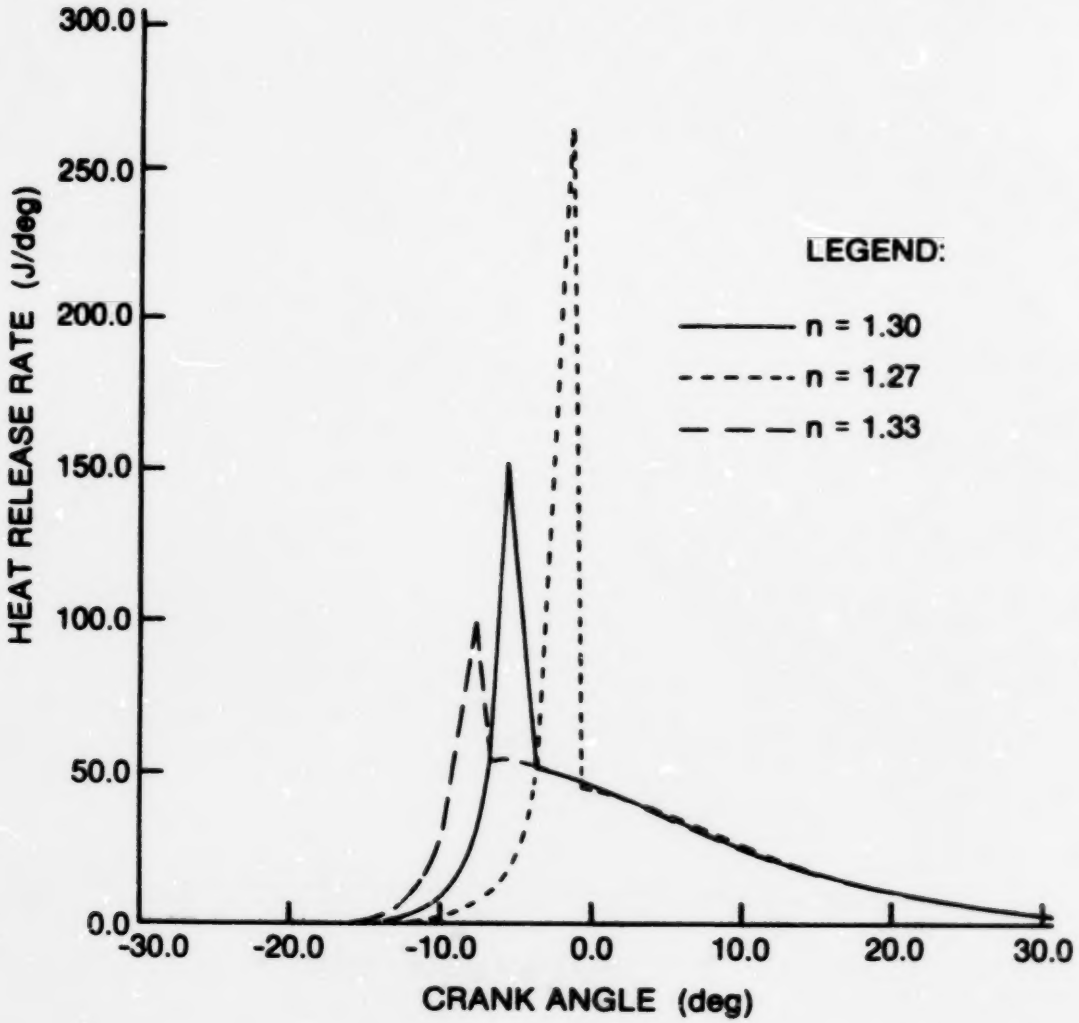


Figure 3 (b). EFFECT OF VARYING THE POLYTROPIC COMPRESSION INDEX: HEAT RELEASE RATE VERSUS CRANK ANGLE.

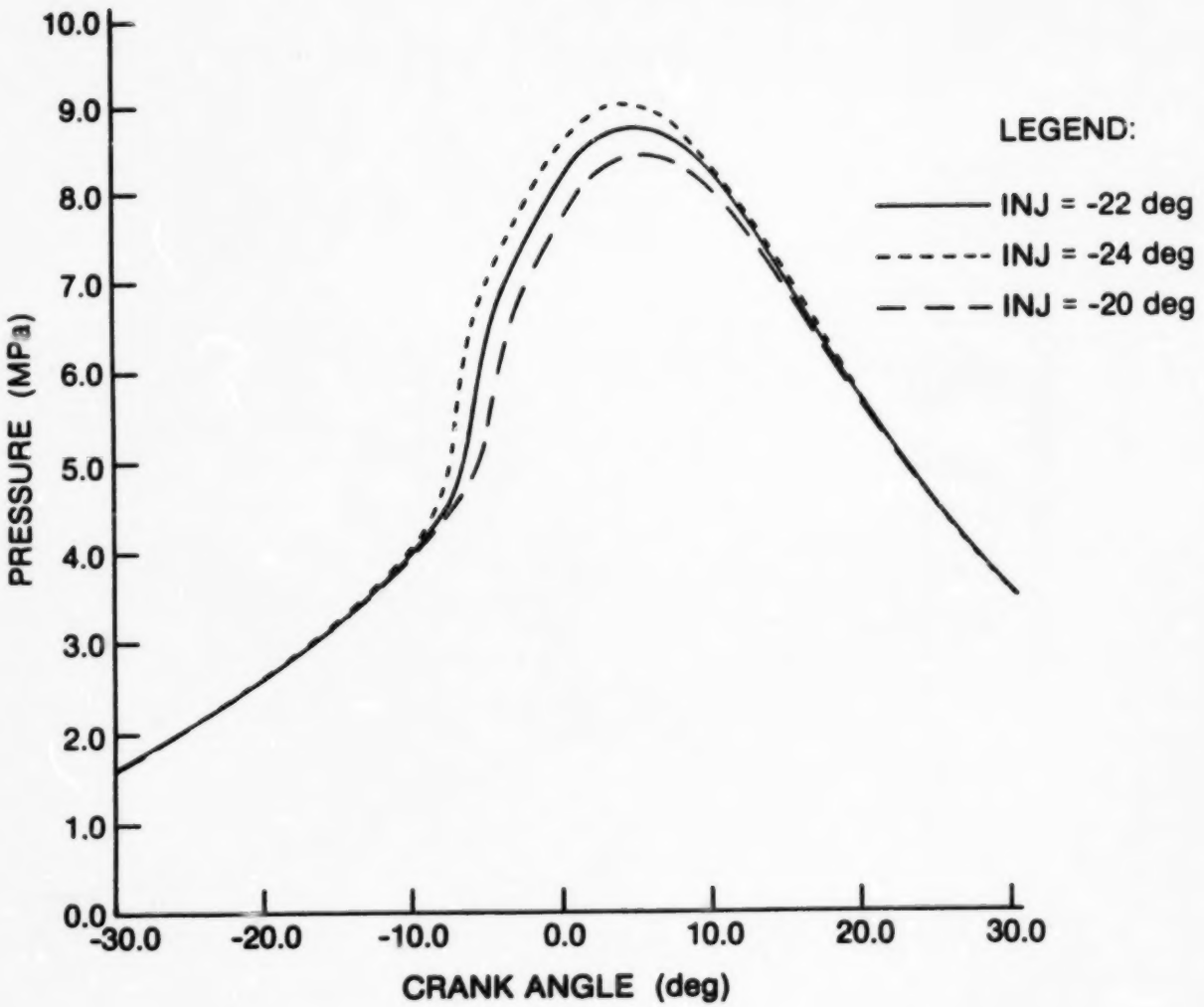


Figure 4 (a). EFFECT OF VARYING THE INJECTION TIMING: CYLINDER PRESSURE VERSUS CRANK ANGLE.

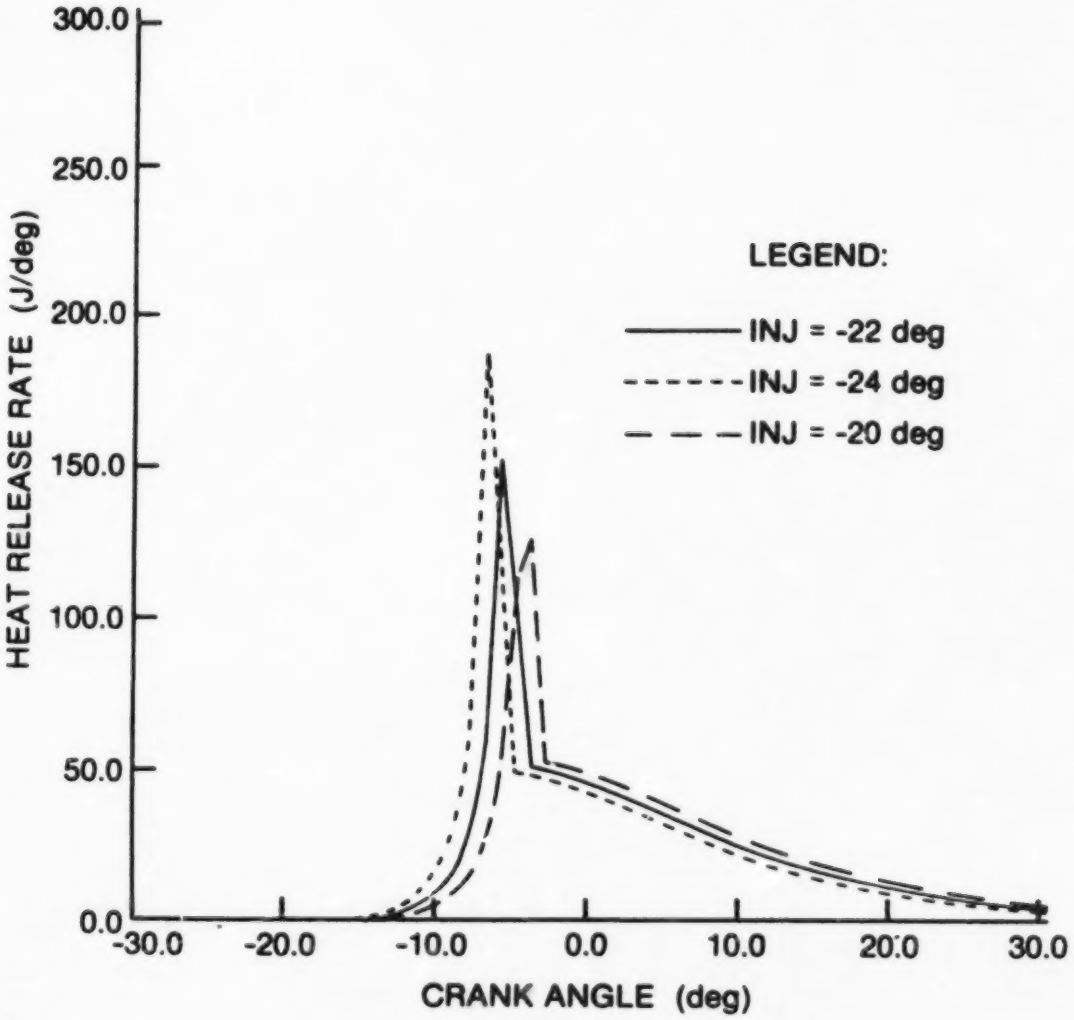


Figure 4 (b). EFFECT OF VARYING THE INJECTION TIMING: HEAT RELEASE RATE VERSUS CRANK ANGLE.

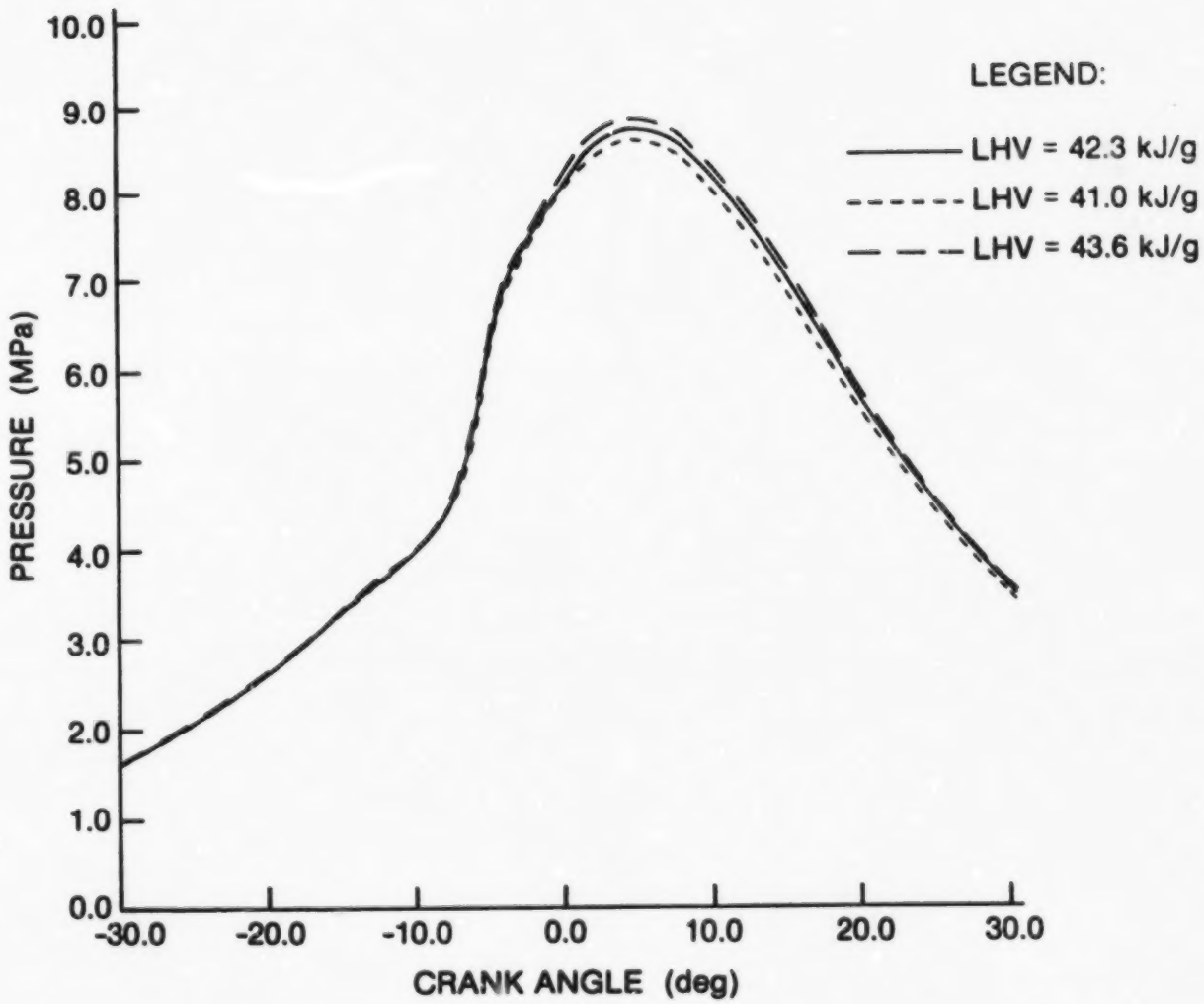


Figure 5 (a). EFFECT OF VARYING THE LOWER HEATING VALUE OF THE FUEL: CYLINDER PRESSURE VERSUS CRANK ANGLE.

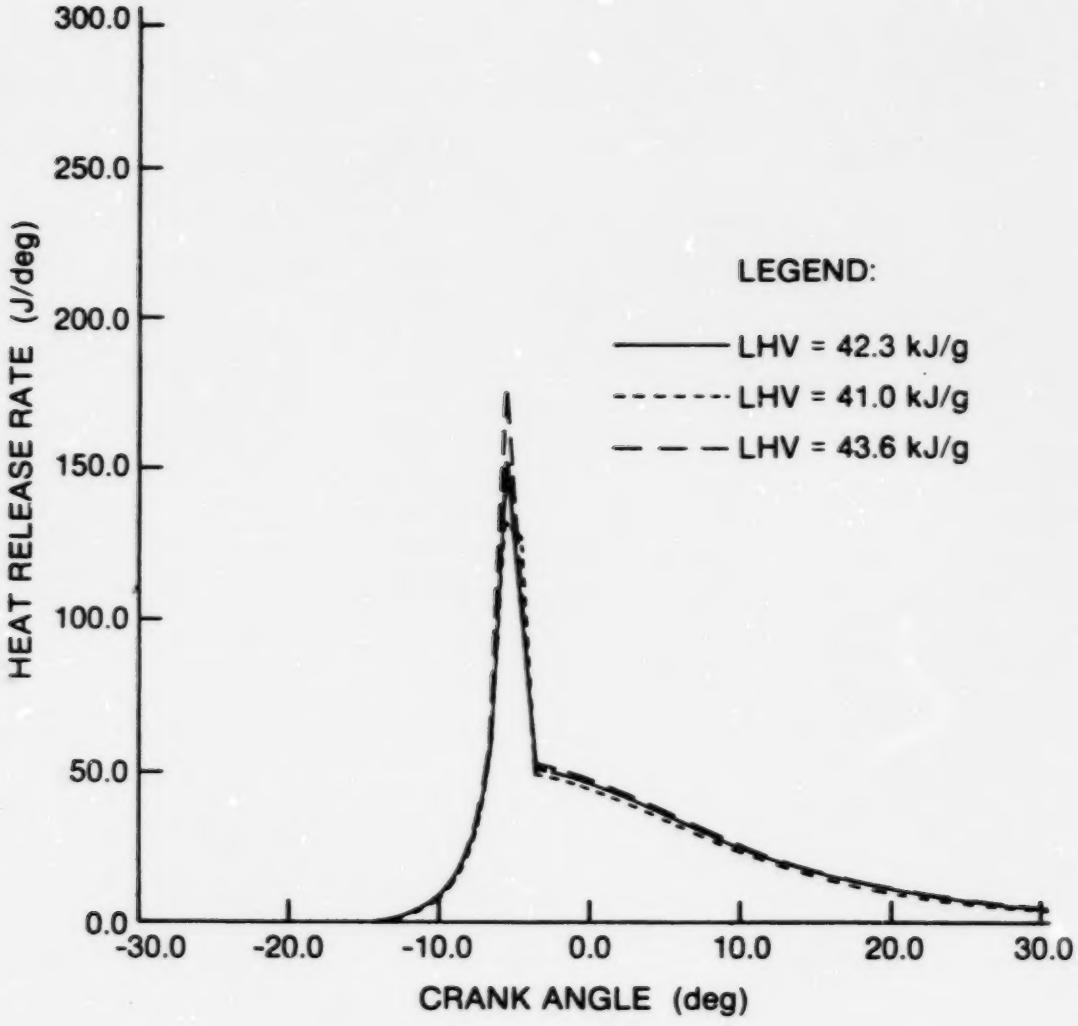


Figure 5 (b). EFFECT OF VARYING THE LOWER HEATING VALUE OF THE FUEL: HEAT RELEASE RATE VERSUS CRANK ANGLE.

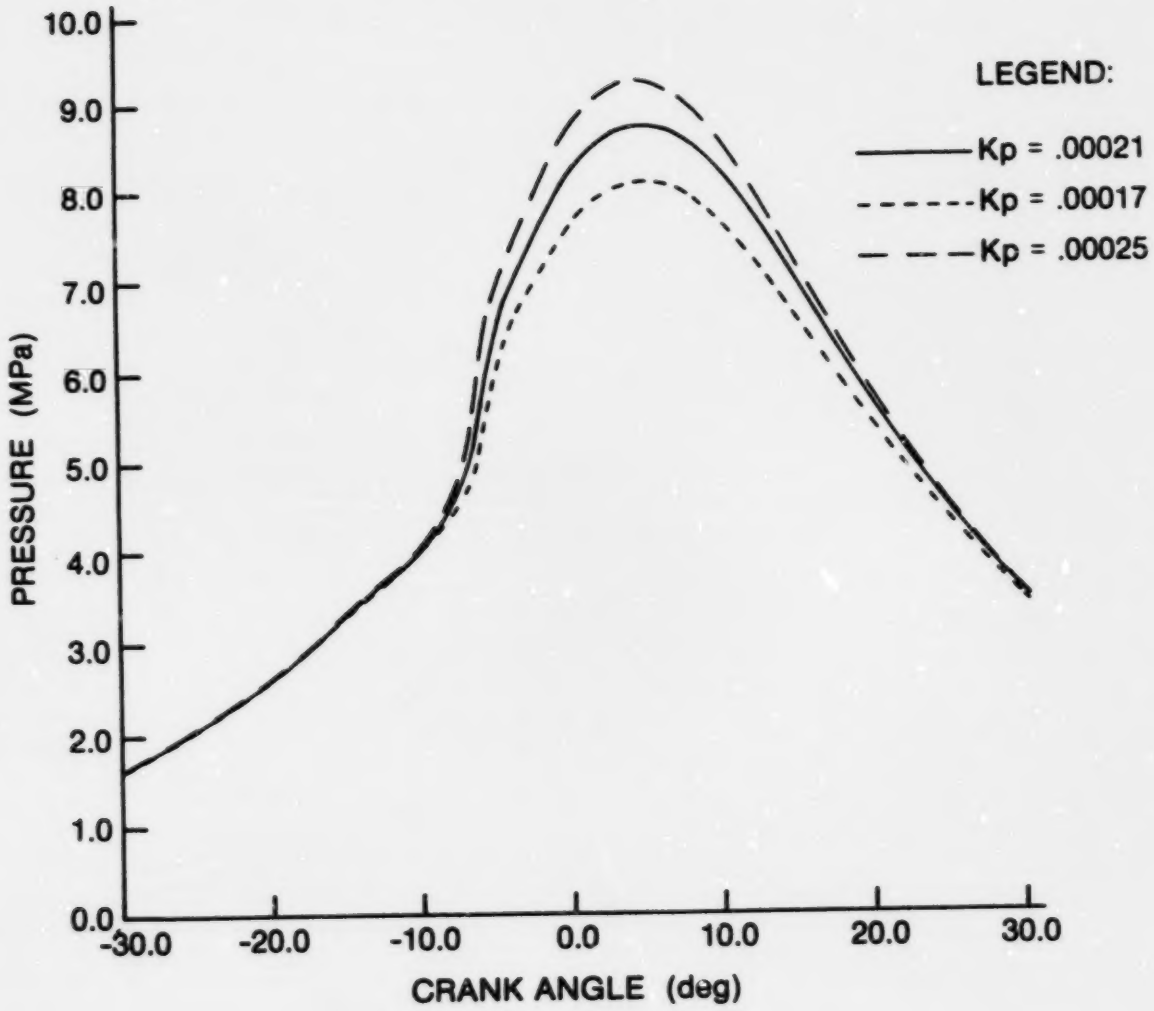


Figure 6 (a). EFFECT OF VARYING THE PREPARATION RATE EQUATION CONSTANT: CYLINDER PRESSURE VERSUS CRANK ANGLE.

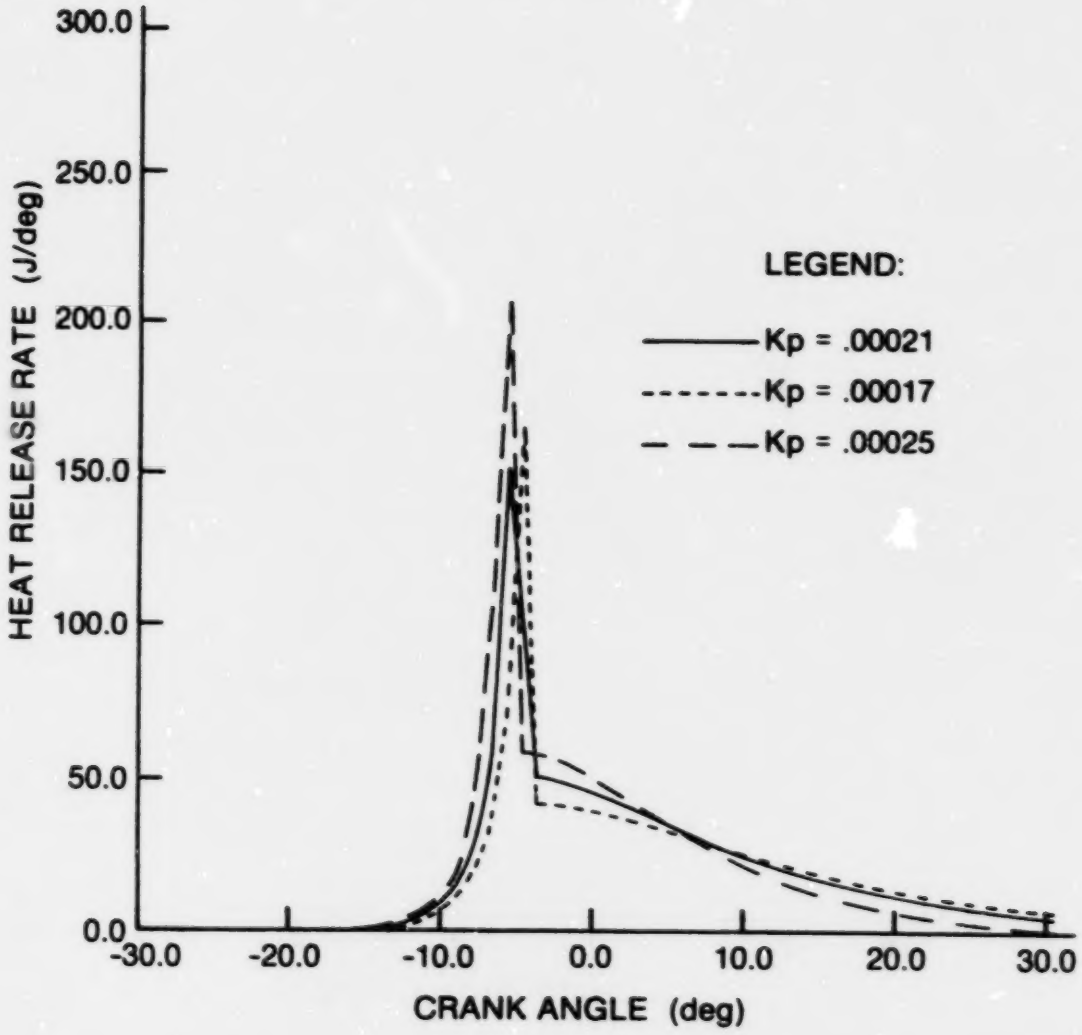


Figure 6 (b). EFFECT OF VARYING THE PREPARATION RATE EQUATION CONSTANT: HEAT RELEASE RATE VERSUS CRANK ANGLE.

3.3.5 Apparent Activation Energy of the Fuel (act)

The quantity exp(-act/T) indicates the fraction of fuel molecules that are capable of reacting at temperature T. The effect of raising the apparent activation energy of the fuel is to increase the ignition delay period (Figure 7). This provides more time for fuel/air mixing to occur. The result is a higher maximum rate of heat release. Figure 7 shows that the maximum rate of heat release increases from 120.3 J/crank angle degree to 218.0 J/degree by increasing the constant act from 14000K to 15000K.

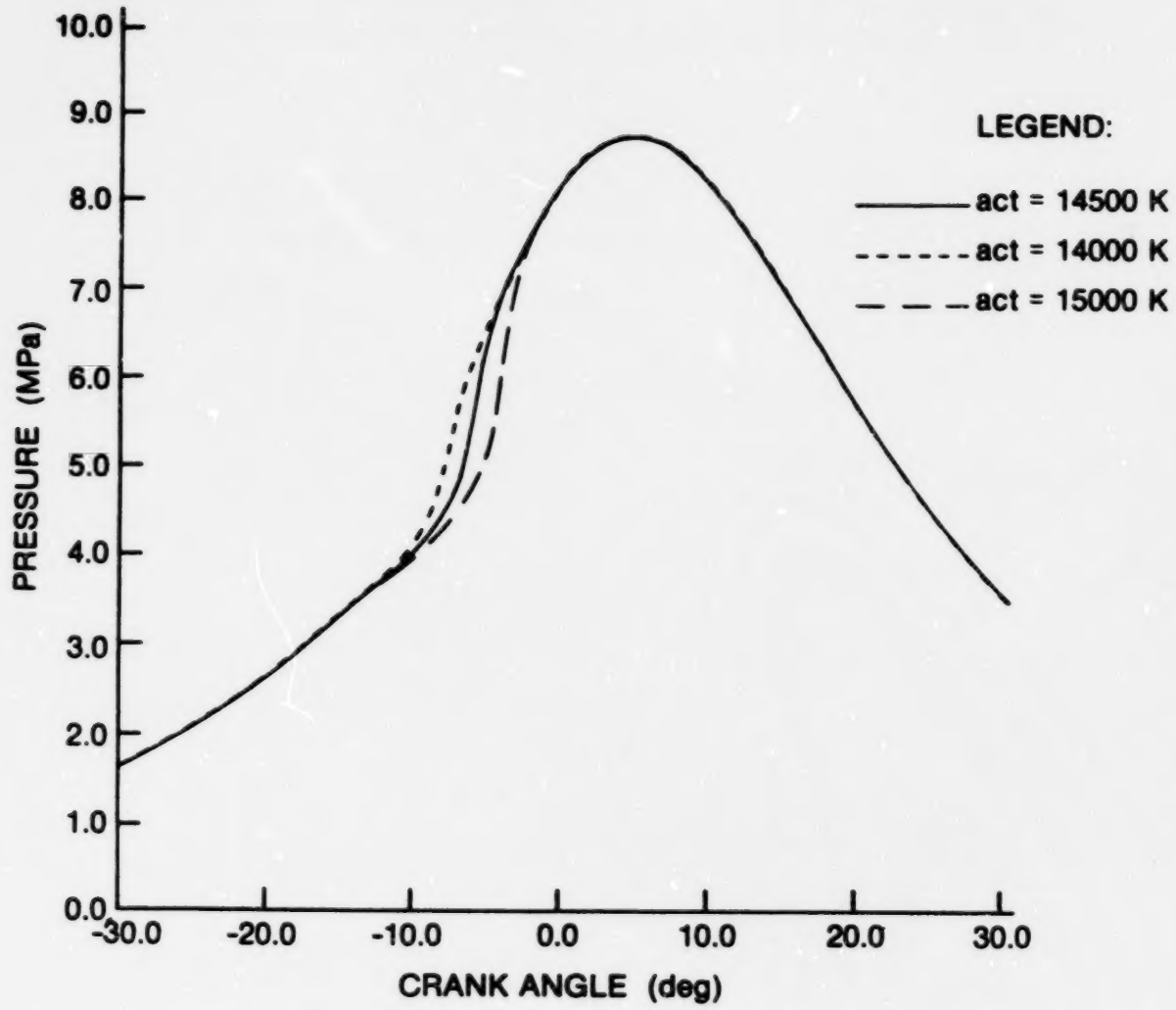


Figure 7 (a). EFFECT OF VARYING THE APPARENT ACTIVATION ENERGY OF THE FUEL: CYLINDER PRESSURE VERSUS CRANK ANGLE.

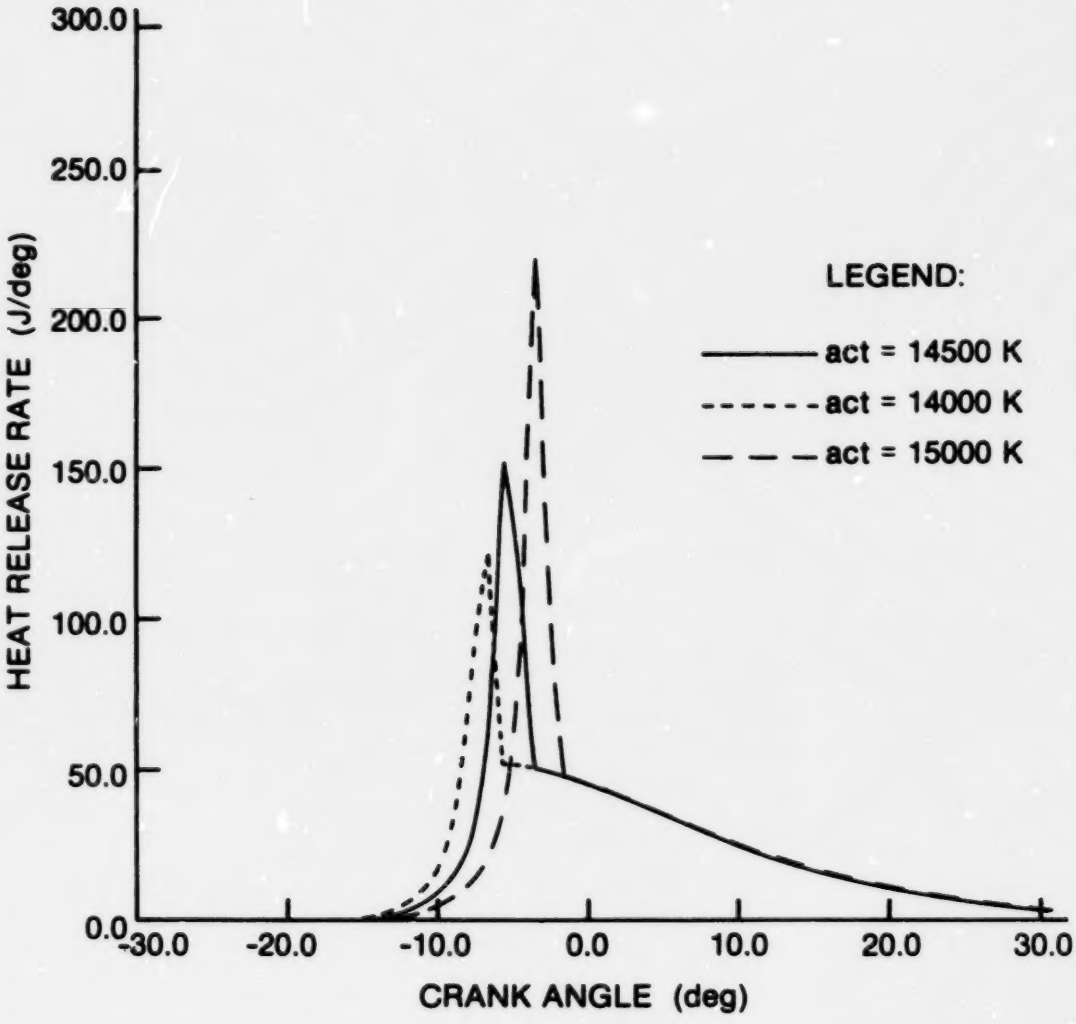


Figure 7 (b). EFFECT OF VARYING THE APPARENT ACTIVATION ENERGY OF THE FUEL: HEAT RELEASE RATE VERSUS CRANK ANGLE.

4.0.0 FUTURE WORK ON COMBUSTION MODELLING

4.1.0 MODEL PERFORMANCE EVALUATION

The single-zone model contains two empirical constants to simulate the combustion process: the preparation rate equation constant and the apparent activation energy of the fuel. In order to be able to predict the effects of future diesel fuels of lower ignition quality on engine performance, one must know how these modelling constants vary as a function of diesel fuel properties. Some work has already been done in this area. Benson and Whitehouse (9) base the preparation rate equation constant on an original empirical value and modify it on the basis of Sauter mean diameter of the fuel droplets injected into the combustion chamber. Whitehouse and Baluswamy (4) propose that variations of ignition quality of fuels be simulated by altering the value of the apparent activation energy in the reaction rate equation. However, only limited investigations of the above hypotheses has been attempted. Moreover, no validation has been done with off-specification and lower ignition quality diesel fuels. Future work on combustion modelling should concentrate on evaluating the above hypotheses with diesel fuels of interest to the Canadian Forces.

CONCLUSIONS

1. An increased understanding of diesel engine combustion has been attained as a result of developing and testing a single-zone model.

2. The single-zone model produces pressure, temperature and heat release diagrams with the correct shape and magnitude.

3. Results of a parametric study performed on the single-zone model are:

   (1) The model correctly indicates the significant effects of varying the fuel injection timing.

   (2) The model predicts that the small variations in heating values of tar sands derived fuels will not be the cause of severe performance problems, and

   (3) A diesel engines' performance is strongly dependent on fuel/air mixing and the ignition quality of the fuel as shown by varying the modelling constants K_p and act respectively.

4. In order to use the single-zone model as a predictive tool, the effect of engine and fuel variables on the empirical constants K_p and act will have to be understood.

RECOMMENDATIONS

1. The diesel fuel properties which significantly affect the preparation rate equation constant and the apparent activation energy should be determined.

2. The capability of the present single-zone model to predict the effects of lower ignition quality diesel fuels should be investigated.

NOMENCLATURE

a	# atoms of carbon in fuel molecule
A	cross-sectional area of combustion chamber (m^2)
act	apparent activation energy of fuel (K)
b	# atoms of hydrogen in fuel molecule
c	radiation heat transfer coefficient ($W/m^2.K^4$)
CA	crank angle (degrees)
CL	crank length (m)
CR	connecting rod (m)
D	bore (m)
h	convection heat transfer coefficient ($W/m^2.K$)
HHV	higher heating value (kJ/g)
k	thermal conductivity (W/m.K)
K_p	preparation rate equation constant
K_r	reaction rate equation constant
LHV	lower heating value (kJ/g)
Δm_f	mass of fuel burned during $\Delta\theta$ (g)
m_i	mass of fuel injected into combustion chamber (g)
m_p	mass of prepared fuel (g)
m_r	mass of fuel that reacts (g)
m_u	mass of unprepared fuel (g)
n	polytropic index of compression

N	engine speed (rpm)
Nu	Nusselt Number
P	cylinder pressure (Pa)
Pr	Prandtl Number
q	heat transfer to combustion chamber walls (W/m^2)
$\hat{R}$	rate of heat release (J/degree)
R	universal gas constant (J/kgmole K)
Re	Reynolds number
T	cylinder temperature (K)
T_w	combustion chamber wall temperature (K)
U	internal energy (J)
V	combustion chamber volume (m^3)
V_c	clearance volume (m^3)
W	work done on piston (J)
X	empirical constant
Y	empirical constant
Z	empirical constant
θ	crank angle (degrees)

BDC	bottom dead centre
TDC	top dead centre
IVC	intake valve closure (degrees)
INJ	start of fuel injection (degrees)
EVO	exhaust valve opening (degrees)

REFERENCES

1. Heywood, J.B., Engine Combustion Modeling - An Overview, Proceedings of the Symposium on Combustion Modeling in Reciprocating Engines, Plenum Press, 1980.

2. Annand, W.J.D., Heat Transfer in the Cylinders of Reciprocating Internal Combustion Engines, Proceedings of the Institution of Mechanical Engineers, Vol. 177, No. 36, 1963.

3. Woschni, G., A Universally Applicable Equation for the Instantaneous Heat Transfer Coefficient in Internal Combustion Engines, Society of Automotive Engineers, paper # 670931, 1967.

4. Whitehouse, N.D. and Baluswamy, N., Calculations of Gaseous Products During Combustion in an Diesel Engine Using a Four Zone Model, Society of Automotive Engineers Paper # 770410, 1977.

5. Oran, E.S. and Boris, J.P., Detailed Modelling of Combustion Systems, Progress in Energy Combustion Sciences, Vol. 7, pp 1-72, 1981.

6. Benson, R.S., Advanced Engineering Thermodynamics, Pergamon Press Limited, 1977 (2nd edition).

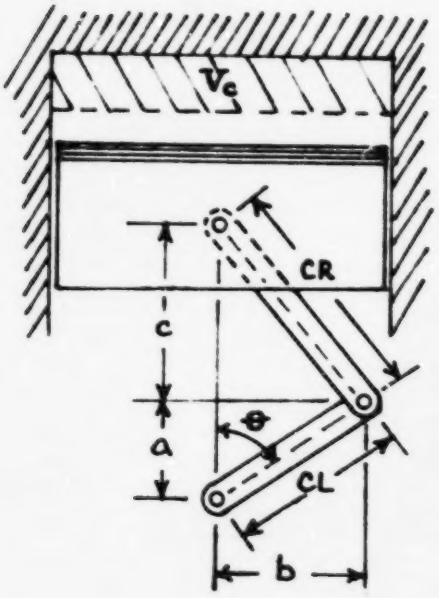
7. Kreith, F., Black, W.Z., Basic Heat Transfer. Harper & Row Publishers, 1980.

8. Garthe, H., Part 1 of Klochner-Humboldt-Deutz paper presented at the VDBUM Seminar held at Braunlage, 1975.

9. Benson, R.S. and Whitehouse, N.D., Internal Combustion Engines, Pergamon Press Limited, 1979.

APPENDIX A

CALCULATION OF CYLINDER VOLUME



$$\text{Volume} = V_c + \left(\frac{\pi\, \text{bore}^2}{4}\right) \quad (CL + CR - a - c)$$

where V_c = clearance volume (m^3)
bore = cylinder diameter (m)
CL = crank length (m)
CR = connecting rod length (m)
θ = crank angle

$a = CL \cos\theta$
$b = CL\,(1-\cos^2\theta)^{\frac{1}{2}}$
$c = CL\,(n^2 - 1 + \cos^2\theta)^{\frac{1}{2}}$
$n = CR/CL$

$$\text{Volume} = V_c + \left(\frac{\pi\, \text{bore}^2}{4}\right) \quad (CL + CR - CL\cos\theta - CL(n^2 - 1 + \cos^2\theta)^{\frac{1}{2}})$$

$$\text{Volume} = V_c + \left(\frac{\pi\, \text{bore}^2}{4}\right) CL\ (1 + n - \cos\theta - (n^2 - \sin^2\theta)^{\frac{1}{2}})$$

APPENDIX B

(Program Listing)

```
01234567890123456789    ** RSX-11M V4.1 **    [101,101]MODEL     - NO PAGE LIMIT
01234567890123456789    ** RSX-11M V4.1 **    FORM #0 - NORMAL HARDWARE FORMS
01234567890123456789    ** RSX-11M V4.1 **    NO IMPLIED FORM FEED
01234567890123456789    ** RSX-11M V4.1 **    JOB CONTAINS 4 FILESPECS
```

```
  CCCCCC        11          000000          11                      11          00
  CCCCCC        11          000000          11                      11          00
  CC          1111        00      00      1111                    1111        00
  CC          1111        00      00      1111                    1111        00
  CC            11        00    0000        11                      11        00
  CC            11        00    0000        11                      11        00
  CC            11        00  00  00        11          ,,,,        11        00
  CC            11        00  00  00        11          ,,,,        11        00
  CC            11        0000    00        11          ,,,,        11      0000
  CC            11        0000    00        11          ,,,,        11      0000
  CC            11        00      00        11            ,,        11        00
  CC            11        00      00        11            ,,        11        00
  CCCCCC      111111        000000        111111          ,,      111111        00
  CCCCCC      111111        000000        111111          ,,      111111        00
```

```
MM      MM      000000      DDDDDDDD      EEEEEEEEEE    LL
MM      MM      000000      DDDDDDDD      EEEEEEEEEE    LL
MMMM  MMMM    00      00    DD      DD    EE            LL
MMMM  MMMM    00      00    DD      DD    EE            LL
MM  MM  MM    00      00    DD      DD    EE            LL
MM  MM  MM    00      00    DD      DD    EE            LL
MM      MM    00      00    DD      DD    EEEEEEEE      LL
MM      MM    00      00    DD      DD    EEEEEEEE      LL
MM      MM    00      00    DD      DD    EE            LL
MM      MM    00      00    DD      DD    EE            LL
MM      MM    00      00    DD      DD    EE            LL
MM      MM    00      00    DD      DD    EE            LL
MM      MM      000000      DDDDDDDD      EEEEEEEEEE    LLLLLLLLLL
MM      MM      000000      DDDDDDDD      EEEEEEEEEE    LLLLLLLLLL
```


```
01234567890123456789    ** RSX-11M V4.1 **    [101,101]MODEL     - NO PAGE LIMIT
01234567890123456789    ** RSX-11M V4.1 **    FORM #0 - NORMAL HARDWARE FORMS
01234567890123456789    ** RSX-11M V4.1 **    NO IMPLIED FORM FEED
01234567890123456789    ** RSX-11M V4.1 **    JOB CONTAINS 4 FILESPECS
```

```
C
C THIS IS A SINGLE ZONE DIESEL ENGINE MODEL
C BASED ON THE METHOD OF BENSON AND WHITEHOUSE
C
C*************************************************
C
      BYTE FILE(30)
      DIMENSION MF(50)
      INTEGER I,J,JMAX,L,K9,INJ
      REAL IVC,EVO,DCA,DCAST,INJST,PAVE
      REAL CR,CL,BORE,VC,ACT,A,B,LHV,R,PI,TS,HHV
      REAL NC,KP,X,Z,KR,RE,NCT,Y
      REAL P,PO,V,VO,T,TO,RPM,TW,MF
      REAL NGAS,NCAHB,NO2,NN2,NH2O,NCO2,NFUEL,NFOLD
      REAL XO2,XN2,XH2O,XCO2,XFUEL,XAIR,PO2
      REAL MMOLD,MI,MU,MP,UDEL,UDELO,PREP,REACTM,REACTH
      REAL UOLD,U,Q,DELMF,W,WTOTAL,VSWEPT,IMEP
      REAL POLD,VOLD,TOLD
      REAL MM,CPAIR,CPN2,CPCO2,CPH2O,CPFUEL,CPM,VAIR,VN2
      REAL VCO2,VH2O,VFUEL,VM,CM,RM,DENM,VELP,REM
      REAL MBURN,INPUT
C
      EXTERNAL VOLUME,HEAT,ENERGY
      TYPE 10
   10 FORMAT(' Enter the data file name: ',$)
      ACCEPT 20,FILE
   20 FORMAT (12A1)
C
      OPEN (UNIT=1,NAME=FILE,TYPE='OLD',
     +      READONLY)
      DO 21 K3=12,1,-1
        IF (FILE(K3).EQ.'.') GOTO 22
   21 CONTINUE
   22 FILE(K3+1)='P'
      OPEN (UNIT=2,NAME=FILE)
      OPEN (UNIT=3,NAME='TDCA.DAT')
      FILE(K3+1)='H'
      OPEN (UNIT=4,NAME=FILE)
      OPEN (UNIT=7,NAME='ENERGY.DAT')
      FILE(K3+1)='S'
      OPEN (UNIT=8,NAME=FILE)
      FILE(K3+1)='F'
      OPEN (UNIT=9,NAME=FILE)
      OPEN (UNIT=10,NAME='GAS.DAT')
      FILE(K3+1)='I'
      OPEN (UNIT=11,NAME=FILE,TYPE='OLD',
     *      READONLY)
C
C*************************************************
C
C INPUT ALL CRANK ANGLES
C
      READ(1,*) IVC,EVO
C
C INPUT ENGINE DIMENSIONS
C
      READ(1,*) CR,CL,BORE,VC
      AA=CR/CL
C
```

```
C INPUT ENGINE CONDITIONS
C
      READ(1,*) PO,TO,TW,RPM
C
C INPUT FUEL PARAMETERS
C
      READ(1,*) A,B,LHV,TS,HHV,VFUEL
C
C INPUT FUEL INJECTION SCHEDULE
C
      READ(1,*) DCAST,INJST,FUEL
      READ(11,40) INJ,JMAX,PAVE,(MF(J),J=1,JMAX)
 40   FORMAT (2I5,F12.8,5(/,10F12.8),/)
C
      I9=0
      DO 42 J=1,JMAX
        IF (MF(J).GE.0.01) I9=I9+1
 42   CONTINUE
C
C CALCULATION OF SAUTER MEAN DIAMETER (MICRONS)
C
      SMD=220.*(VFUEL)**0.215/(PAVE*1.4504E02)**0.458
     *      *(FUEL*RPM*6.614E-02*720./FLOAT(I9))**0.209
C
C  PREPARATION FOR CALCULATION CONSTANTS
C
      X=0.6666666666
      Z=0.40
C
C INPUT MODEL CONSTANTS
C
      READ(1,*) NC,KP,KR,ACT
C
C STORE INPUTS IN THE FILE 'SUMMARY'
C
      FILE(K3+1)='R'
      WRITE(8,1000) FILE
1000  FORMAT (//,T10,'SUMMARY OF INPUT DATA',T50,'RUN # ',20A1,//)
      WRITE(8,1010)
1010  FORMAT (T10,'CRANK ANGLE VALUES',T50,'FUEL PARAMETERS',/)
      WRITE(8,1020) IVC,A*12/B
1020  FORMAT (T10,'IVC=',F5.0,T50,'C/H RATIO=',F5.3)
      WRITE(8,1030) INJ,VFUEL
1030  FORMAT (T10,'INJ=',I3,T50,'FUEL VISCOSITY (cSt)=',F5.3)
      WRITE(8,1040) EVO,HHV
1040  FORMAT (T10,'EVO=',F4.0,T50,'HHV (J/g)=',F6.0,/)
      WRITE(8,1050)
1050  FORMAT (T10,'ENGINE DIMENSIONS',T50,'ENGINE CONDITIONS',/)
      WRITE(8,1060) CR,PO
1060  FORMAT (T10,'CONNECTING ROD LENGTH (m)=',F5.3,
     *        T50,'TRAPPED PRESSURE (Pa)=',F7.0)
      WRITE(8,1070) CL,TO
1070  FORMAT (T10,'CRANK LENGTH (m)=',F5.3,T50,
     *        'TRAPPED TEMPERATURE (K)=',F4.0)
      WRITE(8,1080) BORE,TW
1080  FORMAT (T10,'BORE (m)=',F5.3,T50,
     *        'WALL TEMPERATURE (K)=',F4.0)
      WRITE(8,1090) VC,RPM
1090  FORMAT (T10,'CLEARANCE VOLUME (cu. m)=',E10.4,
```

```
     *          T50,'SPEED (rpm)=',F5.0,/)
          WRITE(8,1100)
 1100     FORMAT (T10,'MODEL CONSTANTS',T50,'INJECTION VALUES',/)
          WRITE(8,1110) NC,INJST
 1110     FORMAT (T10,'NC=',F5.3,T50,'INJECTION STEP=',F4.2)
          WRITE(8,1120) KP,JMAX
 1120     FORMAT (T10,'Kp=',F8.6,T50,'# OF INJECTIONS=',I2)
          WRITE(8,1130) KR,FUEL
 1130     FORMAT (T10,'Kr=',E8.2,,T50,'FUEL INJECTED (g)=',F8.6)
          WRITE(8,1135) ACT
 1135     FORMAT (T10,'ACT=',F6.0,/)
          WRITE(8,1140)
 1140     FORMAT (T25,'FUEL INJECTION SCHEDULE (FRACTION)',/)
          WRITE(8,1150) (MF(J),J=1,JMAX)
 1150     FORMAT (5(T10,7(F6.4,4X),/))
C
C INITIALIZE CONSTANTS
C
          R=8.31
          PI=3.14159265
          K9=0
C
C
C*************************************************
C
C START CALCULATIONS AT INTAKE VALVE CLOSURE
C
          WTOTAL=0.0
          DCA=IVC
          VO=VOLUME(DCA,AA,CL,BORE,VC)
C
C FIND NO. OF MOLES OF GASES IN CYLINDER
C
          NGAS=PO*VO/(R*TO)
          AIR=NGAS
          NN2=0.79*NGAS
          NO2=0.21*NGAS
          NH2O=0.0
          NCO2=0.0
          NCAHB=0.0
          NFUEL=0.0
C
          XO2=NO2/NGAS
          PO2=XO2*PO
          XAIR=1.0
          XCO2=0.0
          XH2O=0.0
          XN2=0.0
          MM=XAIR*29.
C
          V=VO
          P=PO
          T=TO
          WRITE(2,2500) DCA,P*1E-6
          WRITE(3,2500) DCA,T
C
C*************************************************
C
C COMPRESSION STROKE FROM IVC UNTIL INJECTION OCCURS
```

```
C
        NCT=NC-1
 100    IF (DCA.GE.INJ) GOTO 110
          VOLD=V
          POLD=P
          DCA=DCA+DCAST
          IF (DCA.GT.INJ) DCA=INJ
          V=VOLUME(DCA,AA,CL,BORE,VC)
          T=TO*(VO/V)**NCT
          P=PO*(VO/V)**NC
          W=0.5*(P+POLD)*(V-VOLD)
          WTOTAL=WTOTAL+W
          WRITE(2,2500) DCA,P*1E-6
          WRITE(3,2500) DCA,T
        GOTO 100
C
 110    DCA=INJ
C
C*****************************************************
C
C STARTING INJECTION
C
        DCAST=INJST
        I=1
        MI=0.0
        MU=0.0
        MP=0.0
        PREP=0.0
        DELMF=0.0
        MBURN=0.0
        Q=0.0
        QTOTAL=0.0
        REACTM=0.0
        REACTH=0.0
        PRATE=0.0
        PMAX=0.0
        RELMAX=0.0
        CALL ENERGY(T,NO2,NN2,NH2O,NCO2,NFUEL,U)
        CALL ENERGY(TS,NO2,NN2,NH2O,NCO2,NFUEL,US)
        U=U-US
        Y=1-X
C
C*****************************************************
C
 200    IF (DCA.GT.EVO) GOTO 210
C
C INJECT FUEL INTO COMBUSTION CHAMBER
C
          IF (I.GT.JMAX) MF(I)=0.0
          MI=MI+MF(I)*FUEL
          MU=MU+MF(I)*FUEL-PREP*DCAST
          IF (I.LE.JMAX) I=I+1
C
C CALCULATION OF FUEL PREPARATION RATE (G/DEGREE)
C
          PREP=KP*(MI**Y)*(MU**X)*(PO2**Z)
          MP=MP+(PREP-REACTM)*DCAST
          IF (MP.LT.MU) GOTO 220
          MP=MU
```

```
          PREP=MP/DCAST
 220      CONTINUE
C
          DCAOLD=DCA
          UOLD=U
          VOLD=V
          POLD=P
          TOLD=T
          WRITE(2,2500) DCA,P*1E-6
          WRITE(3,2500) DCA,T
          WRITE(4,2501) DCA,PREP,REACTM
          WRITE(9,2502) DCA,PO2*1E-6,MP,EXP(-ACT/T),1./RPM,1./SQRT(T)
     *                  ,REACTM
          WRITE(10,*) DCA,NGAS,NO2,NN2,NH2O,NCO2,XO2
          WRITE(7,*) DCA,T,U,Q,W,REACTH*DCAST,K9
C
C NEW CRANK ANGLE
C
          DCA=DCA+DCAST
          IF (DCA.GE.EVO) GOTO 210
          V=VOLUME(DCA,AA,CL,BORE,VC)
C
C CALCULATION OF MOLES OF GASES
C
          NCAHB=DELMF/(12.*A+B)
          NO2=NO2-NCAHB*(A+B*0.25)
          NFUEL=(MI-MBURN)/(12.*A+B)
          NCO2=NCO2+NCAHB*A
          NH2O=NH2O+NCAHB*B*0.5
          NGAS=NGAS+NCAHB*B*0.25
C
C CALCULATION OF MOLE FRACTIONS (NO UNITS)
C
          XAIR=100.*XO2/21.
          XO2=NO2/NGAS
          XCO2=NCO2/NGAS
          XN2=1.0-XAIR-XCO2-XH2O
          PO2=XO2*P
C
C CALCULATION OF THE MASS OF MIXTURE (G/GMOLE)
C
          MM=XAIR*29.+XN2*28.+XCO2*44.+XH2O*18.
C
C CALCULATION OF GAS CONSTANT OF MIXTURE (J/KG-K)
C
          RM=1000.*R/MM
C
C CALCULATION OF REACTION RATE (G/DEGREE)
C
          REACTM=KR*PO2*MP*EXP(-ACT/T)/(RPM*SQRT(T))
          REACTH=REACTM*LHV
          DELMF=REACTM*DCAST
          IF (DELMF.LE.MP) GOTO 230
          DELMF=MP
          REACTM=DELMF/DCAST
          REACTH=REACTM*LHV
 230      CONTINUE
          MBURN=MBURN+DELMF
C
```

```
      DELT=TOLD*((VOLD/V)**NCT-1)
      K9=1
C
C*************************************************************
C
C TEMPERATURE ITERATION
C
 240  IF (K9.GT.30) GOTO 250
 260  T=T+DELT
      P=NGAS*R*T/V
      TBAR=(T+TOLD)*0.5
      DCABAR=(DCA+DCAOLD)*0.5
C
C CALCULATION OF SPECIFIC HEATS (Chu/LB-C)
C
      CPAIR=0.224+0.471E-4*TBAR
      CPN2=0.233+0.446E-4*TBAR-0.004E-8*(TBAR**2)
      CPCO2=0.141+2.363E-4*TBAR-8.057E-8*(TBAR**2)
      CPH2O=0.479-0.807E-4*TBAR+15.86E-8*(TBAR**2)
C
      CPM=(XAIR*29.*CPAIR+XN2*28.*CPN2+
     +     XCO2*44.*CPCO2+XH2O*18.*CPH2O)/MM
C
C CALCULATION OF DYNAMIC VISCOSITIES (LBM/FT-SEC)
C
      VAIR=3.16E-7*(TBAR**0.645)
      VN2=3.07E-7*(TBAR**0.645)
      VCO2=2.49E-7*(TBAR**0.645)
      VH2O=2.19E-7*(TBAR**0.645)
C
      VM=(XAIR*5.385*VAIR+XN2*5.292*VN2+XCO2*6.633*VCO2
     +     +XH2O*4.243*VH2O)/
     +     (XAIR*5.385+XN2*5.292+XCO2*6.633+XH2O*4.243)
C
C PR=0.7 APPROXIMATELY
C
C CONDUCTIVITY OF MIXTURE (Chu/FT-SEC-C)
C
      CM=VM*CPM/0.70
C
C CALCULATION OF MIXTURE DENSITY (KG/CU M)
C
      DENM=(POLD+P)/(2.*RM*TBAR)
C
C CALCULATION OF PISTON MEAN VELOCITY (M/S)
C
      VELP=2.*(2.*CR)*RPM/60.
C
C CALCULATION OF REYNOLDS NUMBER
C
      REM=(DENM*VELP*BORE)/(VM*0.454*3.28)
C
      CALL HEAT(TBAR,TW,REM,CM,BORE,DCAST,RPM,V,Q)
      W=0.5*(P+POLD)*(V-VOLD)
C
C ENERGY BALANCE
C
      CALL ENERGY (T,NO2,NN2,NH2O,NCO2,NFUEL,U)
      CALL ENERGY (TS,NO2,NN2,NH2O,NCO2,NFUEL,US)
```

```
          U=U-US
          UDEL=UOLD-U+REACTH*DCAST-Q-W
          IF (ABS(UDEL/U).LE.0.001) GOTO 300
          IF (K9.GT.1) GOTO 310
C FIRST ITERATION
          DELT=(REACTH*DCAST-Q-W)/(29.064*NGAS)
          TS      LD
          GOTO 320
C SUBSEQUENT ITERATIONS
 310      DELT=(TSTAR-(UDELO*(T-TSTAR))/(UDEL-UDELO))-T
          TSTAR=T
 320      UDELO=UDEL
          K9=K9+1
          GOTO 240
 250      CONTINUE
          STOP
C
C*************************************************
C
 300      CONTINUE
C
          WTOTAL=WTOTAL+W
          QTOTAL=QTOTAL+Q
          IF (P.LE.PMAX) GOTO 400
          PMAX=P
          LOCMAX=DCA
 400      IF ((P-POLD)/DCAST.LE.PRATE) GOTO 410
          PRATE=(P-POLD)/DCAST
          LOCRAT=DCA
 410      IF (REACTH.LE.RELMAX) GOTO 420
          RELMAX=REACTH
          LOCREL=DCA
 420      GOTO 200
 210      CONTINUE
C
C*************************************************
C
C END OF CLOSED PERIOD
C
C

        PBURN=100.*MBURN/MI
        RATIO=29.*AIR/MI
        INPUT=MI*HHV
        PWORK=100.*WTOTAL/INPUT
        PHEAT=100.*QTOTAL/INPUT
C
C OUTPUT DATA INTO FILE 'SUMMARY.DAT'
C
        WRITE(8,1500)
 1500   FORMAT (//,T30,'SUMMARY OF TEST RESULTS',/)
        WRITE(8,1510)
 1510   FORMAT (T10,'QUANTITY',T50,'PERCENT OR LOCATION',/)
        WRITE(8,1520) RATIO
 1520   FORMAT (T10,'AIR/FUEL RATIO=',F5.2)
        WRITE(8,1525) SMD
 1525   FORMAT (T10,'FUEL SAUTER MEAN DIAMETER (microns)=',F6.3,/)
        WRITE(8,1530) MBURN,PBURN
 1530   FORMAT (T10,'FUEL BURNED (g)=',F8.6,T58,F5.1)
```

```
      WRITE(8,1540) WTOTAL,PWORK
 1540 FORMAT (T10,'WORK (J)=',F5.1,T58,F5.1)
      WRITE(8,1550) QTOTAL,PHEAT
 1550 FORMAT (T10,'HEAT (J)=',F5.1,T58,F5.1,/)
      WRITE(8,1560) PMAX*1E-6,LOCMAX
 1560 FORMAT (T10,'MAX. PRES. (MPa)=',F6.3,T58,I3)
      WRITE(8,1570) PRATE*1E-06,LOCRAT
 1570 FORMAT (T10,'MAX. dP/dCA (MPa/CA)=',F6.3,T58,I3)
      WRITE(8,1580) RELMAX,LOCREL
 1580 FORMAT (T10,'MAX. H.R. RATE (J/CA)=',F7.3,T58,I3)
C
 2500 FORMAT (2G13.5)
 2501 FORMAT (G13.5,F8.6,3X,F8.6)
 2502 FORMAT (G13.5,F6.3,5(3X,F8.6))
C
      CLOSE (UNIT=1)
      CLOSE (UNIT=2,DISP='SAVE')
      CLOSE (UNIT=3,DISP='DELETE')
      CLOSE (UNIT=4,DISP='SAVE')
      CLOSE (UNIT=7,DISP='DELETE')
      CLOSE (UNIT=8,DISP='SAVE')
      CLOSE (UNIT=9,DISP='SAVE')
      CLOSE (UNIT=10,DISP='DELETE')
      CLOSE (UNIT=11)
      END
```

```
C
C THIS SUBROUTINE CALCULATES THE INTERNAL ENERGY OF THE
C COMBUSTION CHAMBER CONTENTS
C
C SEE 'INTERNAL COMBUSTION ENGINES'
C BY BENSON AND WHITEHOUSE
C
      SUBROUTINE ENERGY (T,NO2,NN2,NH2O,NCO2,NFUEL,E)
      REAL R,UO2,UN2,UH2O,UCO2,UFUEL
      REAL E,T,NO2,NN2,NH2O,NCO2,NFUEL
C
C UNIVERSAL GAS CONSTANT IN J/GMOL-K
C
      R=8.31
C
      IF (T.LE.5000.) GOTO 5
      WRITE(10,*) T
      STOP
C
C INTERNAL ENERGY OF EACH GAS (JOULES)
C
 5    UO2=NO2*(R*(3.25304*T+(6.52350E-4)*T**2-(1.49524E-7)*
     +       T**3+(1.53897E-11)*T**4-T))
      UN2=NN2*(R*(3.34435*T+(2.94260E-4)*T**2+(1.95300E-9)*
     +       T**3-(6.57470E-12)*T**4-T))
      UH2O=NH2O*(R*(3.74292*T+(5.65590E-4)*T**2+(4.95240E-8)*
     +       T**3-(1.81802E-11)*T**4-T))
      UCO2=NCO2*(R*(3.09590*T+(2.73114E-3)*T**2-(7.88542E-7)*
     +       T**3+(8.66002E-11)*T**4-T))
      UFUEL=NFUEL*(R*(-0.71993*T+4.6426E-2*T**2-(1.68385E-5)*
     +       T**3+2.67009E-9*T**4-T))
C
C THE INTERNAL ENERGY
C
      E=UO2+UN2+UH2O+UCO2+UFUEL
      RETURN
      END
```

```
C
C THIS SUBROUTINE CALCULATES THE HEAT TRANSFER TO THE
C COMBUSTION CHAMBER WALLS DURING A CRANK ANGLE INCREMENT.
C
C METHOD DEVELOPED BY W.J.D. ANNAND
C SEE REFERENCE FILE 967
C
      SUBROUTINE HEAT (T,TW,REM,CM,BORE,DCAST,RPM,V,Q)
      REAL T,TW,REM,CM,BORE,DCAST,RPM,V,Q
      REAL PI,QRATE,A,B,C,TIME,AREA
C
C HEAT TRANSFER SURFACE AREA (SQUARE METRES)
C
      DATA PI/3.14159265/
      AREA=4.0*V/BORE+PI*(BORE**2)**0.5
C
      A=0.60
      B=0.70
      C=3.0E-11
C
C CALCULATION OF QRATE IN (Chu/S-SQ. FT.)
C
      QRATE=A*CM*(REM**B)*(T-TW)/BORE+C*(T**4-TW**4)
C
C CALCULATION OF TIME
C
      TIME=DCAST/(60.0*RPM)
C
C HEAT TRANSFER DURING THE INTERVAL (JOULES)
C
      Q=QRATE*AREA*20433.24*TIME
C
      RETURN
      END
```

```
C
C THIS SUBROUTINE CALCULATES THE COMBUSTION CHAMBER
C VOLUME AS A FUNCTION OF CRANK ANGLE
C
      FUNCTION VOLUME (DCA,AA,CL,BORE,VC)
C
      PI=3.14159265
      RAD=DCA*PI/180.
      BB=SQRT(AA**2-SIN(RAD)**2)
      IF (DCA.NE.90) GOTO 10
      CC=CL*(1+AA-BB)
      GOTO 20
 10   CC=CL*(1+AA-BB-COS(RAD))
C
 20   VOLUME=VC+0.25*CC*PI*BORE**2
      RETURN
      END
```

APPENDIX C

INPUT FILE REQUIRED TO RUN PROGRAM

line 1 intake valve closure (°CA), exhaust valve opening (°CA).

line 2 connecting rod length (m), crank length (m), bore (m), clearance volume (m).

line 3 trapped pressure (Pa), trapped temperature (K), wall temperature (K), engine speed (rpm)

line 4 # of carbon atoms in fuel molecule, # of hydrogen atoms in fuel molecule, LHV of fuel (J/g), reference temperature of LHV and HHV of fuel (K), HHV of fuel (J/g).

line 5 program step size during compression stroke (°CA), program step size during combustion portion of cycle (°CA).

line 6 total fuel injected (g/cycle).

line 7 polytropic compression index, preparation rate equation constant, reaction rate equation constant, activation energy (K).

FUEL INJECTION SCHEDULE

line 1 start of fuel injection (°CA), number of injections, average net injection pressure (MPa)

line 2 fraction of fuel injected during each crank angle interval from start to end of injection

UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall document is classified)

1. ORIGINATING ACTIVITY
Defence Research Establishment Ottawa
Department of National Defence
Ottawa, Ontario, K1A 0Z4, Canada

2a. DOCUMENT SECURITY CLASSIFICATION
Unclassified

2b. GROUP

3. DOCUMENT TITLE
DEVELOPMENT OF A SINGLE-ZONE DIRECT INJECTION DIESEL ENGINE MODEL

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)
Technical Note

5. AUTHOR(S) (Last name, first name, middle initial)
NEILL, W.S. and WEBSTER, G.D.

6. DOCUMENT DATE
August 1984

7a. TOTAL NO OF PAGES
54

7b. NO OF REFS
9

8a. PROJECT OR GRANT NO.
25B10

8b. CONTRACT NO.

9a. ORIGINATOR'S DOCUMENT NUMBER(S)
DREO TN 84-12

9b. OTHER DOCUMENT NO.(S) (Any other numbers that may be assigned this document)

10. DISTRIBUTION STATEMENT

11. SUPPLEMENTARY NOTES

12. SPONSORING ACTIVITY

13. ABSTRACT

A computer model is being developed at DREO to simulate the combustion process in diesel engines, and in particular to acquire the ability to predict the effects of future lower grade fuels on diesel engine performance. A baseline thermodynamic model has been completed. Two rate equations developed by Whitehouse and Way, describe the transient fuel/air mixing and reaction kinetic processes. A parametric study was initiated to obtain a better understanding of the sensitivity of fuel parameters and modelling constants on the model's output. It was found that the model produces pressure and heat release diagrams with the correct shape and magnitude. The model predicted the correct trending in all cases studied. In order to use the model as a predictive took, the effect of engine and fuel variables on the modelling constants will have to be determined.

DSIS

77-465

UNCLASSIFIED
Security Classification

KEY WORDS

diesel engine
simulation
thermodynamic
single-zone

INSTRUCTIONS

1 ORIGINATING ACTIVITY: Enter the name and address of the organization issuing the document.

2a DOCUMENT SECURITY CLASSIFICATION: Enter the overall security classification of the document including special warning terms whenever applicable.

2b GROUP: Enter security reclassification group number. The three groups are defined in Appendix 'M' of the DRB Security Regulations.

3 DOCUMENT TITLE: Enter the complete document title in all capital letters. Titles in all cases should be unclassified. If a sufficiently descriptive title cannot be selected without classification, show title classification with the usual one-capital-letter abbreviation in parentheses immediately following the title.

4 DESCRIPTIVE NOTES: Enter the category of document, e.g. technical report, technical note or technical letter. If appropriate, enter the type of document, e.g. interim, progress, summary, annual or final. Give the inclusive dates when a specific reporting period is covered.

5. AUTHOR(S): Enter the name(s) of author(s) as shown on or in the document. Enter last name, first name, middle initial. If military, show rank. The name of the principal author is an absolute minimum requirement.

6 DOCUMENT DATE: Enter the date (month, year) of Establishment approval for publication of the document.

7a TOTAL NUMBER OF PAGES: The total page count should follow normal pagination procedures, i.e., enter the number of pages containing information.

7b NUMBER OF REFERENCES: Enter the total number of references cited in the document.

8a PROJECT OR GRANT NUMBER: If appropriate, enter the applicable research and development project or grant number under which the document was written.

8b. CONTRACT NUMBER: If appropriate, enter the applicable number under which the document was written.

9a. ORIGINATOR'S DOCUMENT NUMBER(S): Enter the official document number by which the document will be identified and controlled by the originating activity. This number must be unique to this document.

9b OTHER DOCUMENT NUMBER(S): If the document has been assigned any other document numbers (either by the originator or by the sponsor), also enter this number(s).

10 DISTRIBUTION STATEMENT: Enter any limitations on further dissemination of the document, other than those imposed by security classification, using standard statements such as

(1) "Qualified requesters may obtain copies of this document from their defence documentation center."

(2) "Announcement and dissemination of this document is not authorized without prior approval from originating activity."

11. SUPPLEMENTARY NOTES: Use for additional explanatory notes.

12. SPONSORING ACTIVITY: Enter the name of the departmental project office or laboratory sponsoring the research and development. Include address.

13. ABSTRACT: Enter an abstract giving a brief and factual summary of the document, even though it may also appear elsewhere in the body of the document itself. It is highly desirable that the abstract of classified documents be unclassified. Each paragraph of the abstract shall end with an indication of the security classification of the information in the paragraph (unless the document itself is unclassified) represented as (TS), (S), (C), (R), or (U).

The length of the abstract should be limited to 20 single-spaced standard typewritten lines; 7½ inches long.

14. KEY WORDS: Key words are technically meaningful terms or short phrases that characterize a document and could be helpful in cataloging the document. Key words should be selected so that no security classification is required. Identifiers, such as equipment model designation, trade name, military project code name, geographic location, may be used as key words but will be followed by an indication of technical context.

POOR

QUALITY

ORIGINAL